Applicability of the Taylor-Green-Kubo formula in particle diffusion theory

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Diffusion coefficients of particles can be defined as time integrals over velocity correlation functions, or as mean square displacements divided by time. In the present paper it is demonstrated that these two definitions are not equivalent. An exact relation between mean square displacements and velocity correlations is derived. As an example of the applicability of these results so-called drift coefficients of energetic particles are discussed. It is explained why different previous approaches in drift theory provided contradicting results.

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I. INTRODUCTION

A fundamental problem in physics is the stochastic propagation of particles in two or three dimensions. A prominent example is the motion of a *Brownian particle* described by Brown and Einstein (see Refs. [1] and [2]). A more general discussion of the stochastic motion of particles in physics and astronomy was presented by Chandrasekhar (see Ref. [3]). Another example is the propagation of energetic charged particles in magnetized plasmas (see, e.g., Refs. [4] and [5]). In the latter case the particles are scattered due to complicated interactions with turbulent electric and magnetic fields. Such fields are usually superposed by a mean magnetic field. The latter field breaks the symmetry of the physical system and, thus, there is a preferred direction of the particles; i.e., the particles prefer to propagate along the mean magnetic field (see, e.g., Ref. [6]). Although there is a preferred direction, particles are also scattered across the mean magnetic field.

An example of energetic particles propagating through a plasma is the motion of charged particles in fusion devices (see, e.g., Refs. [7] and [8]). In this context, the interaction of alpha particles or accelerated ion beams with the turbulence in a *tokamak* is a topic of great interest. Another example is the motion of energetic particles such as cosmic rays through the interplanetary or interstellar plasma (see, e.g., Refs. [9] and [10]).

Due to the stochastic motion, one can use *mean square displacements* of particle trajectories to describe the propagation. For example, in the x direction we can assume that $\langle (\Delta x)^2 \rangle \sim t^\alpha$ with $\Delta x = x(t) - x(t_0)$. Here we used the ensemble average operator $\langle \ldots \rangle$ and the initial time t_0. This corresponds to an increase of the uncertainty to find the particle at a position in space if time t passes. The parameter α can be used to characterize the particle motion. For example, we have by definition *subdiffusion* if $\alpha < 1$, *diffusion* if $\alpha = 1$, and a *superdiffusive motion* if $\alpha > 1$. Although nondiffusive transport has been discussed more and more in the recent years (see, e.g., Refs. [11–16]), it is still a standard assumption that particles propagate diffusively. The latter process is also known as *normal* or *Markovian diffusion* (named after the Russian mathematician A. A. Markov).

If the particle motion is diffusive, the three dimensional propagation of the particle can be described by a diffusion tensor

$$(\kappa_{ij}) = \begin{Bmatrix} \kappa_{xx} & \kappa_{xy} & \kappa_{xz} \\ \kappa_{yx} & \kappa_{yy} & \kappa_{yz} \\ \kappa_{zx} & \kappa_{zy} & \kappa_{zz} \end{Bmatrix}, \tag{1}$$

where we used a *Cartesian system of coordinates*. If we assume that there is a mean magnetic field pointing in the z direction, we can call $\kappa_{zz} \equiv \kappa_\parallel$ the parallel diffusion coefficient, κ_{xx} and κ_{yy} the perpendicular diffusion coefficients, and κ_{ij} with $i \neq j$ the off-diagonal elements. A strong simplification can be achieved if we assume axisymmetry with respect to the mean magnetic field. This special case is considered later in the paper.

In the literature one can find two different definitions of the diffusion coefficient. If the transport is diffusive ($\alpha = 1$) we can define a diffusion coefficient in the ij direction as

$$\kappa_{ij}^{\mathrm{MSD}} = \lim_{t\to\infty} \frac{\langle \Delta x_i \Delta x_j \rangle}{2t}. \tag{2}$$

In this case the diffusion coefficient is defined by using the *mean square displacements* (MSDs) of all possible particle trajectories. Alternatively, one can find the following formula in the literature:

$$\kappa_{ij}^{\mathrm{VCF}} = \int_0^\infty dt \langle v_i(t) v_j(0) \rangle. \tag{3}$$

In this case the diffusion coefficient is defined as a time integral over the *velocity correlation function* (VCF). This formula is based on the work of Taylor, Green, and Kubo (see Refs. [17–19]) and is, therefore, known as *Taylor-Green-Kubo* (TGK) or *Kubo* formula.

In the present paper it will be demonstrated that Eqs. (2) and (3) are not equivalent for the off-diagonal elements of the diffusion tensor (1); i.e., $\kappa_{ij}^{\mathrm{MSD}} \neq \kappa_{ij}^{\mathrm{VCF}}$ if $i \neq j$. As an example we consider so-called *drift coefficients* in the theory of solar modulation where a disagreement between different previous results had been found in the recent years (see, e.g., Ref. [20] and references therein).

II. EXACT RELATION BETWEEN MEAN SQUARE DISPLACEMENTS AND VELOCITY CORRELATIONS

We start our investigation with Eq. (2) which can be written as $\langle \Delta x_i \Delta x_j \rangle = 2t\kappa_{ij}^{\mathrm{MSD}}$. Usually it is assumed that

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this relation is only correct in the formal limit $t \to \infty$ since it needs a certain time before the particle approaches the stable (diffusive?) regime. More general is a full time dependent description of the transport. In the following we derive general relations for time dependent diffusion coefficients. The asymptotic limit $t \to \infty$ is only considered for some examples and to relate our new results to previously derived relations. To achieve a full time dependent description, we can define a *running diffusion coefficient* as

$$D_{ij}(t) := \frac{1}{2}\frac{d}{dt}\langle \Delta x_i \Delta x_j^* \rangle, \tag{4}$$

where we allowed complex valued positions which is useful if we allow complex valued fields causing the scattering of the particles. Furthermore, we have used the notation x_j^* for *complex conjugate*. If the particle motion is indeed diffusive, the *running diffusion coefficient* becomes constant in the (formal) limit $t \to \infty$ and Eqs. (2) and (4) are equivalent. The displacement used above can be related to the i component of the particle velocity vector v_i via

$$\Delta x_i(t) = \int_{t_0}^{t} d\tau\, v_i(\tau) \tag{5}$$

with $t > t_0$. Therewith, we can easily write the mean square displacements as

$$\langle \Delta x_i \Delta x_j^* \rangle = \int_{t_0}^{t} d\tau \int_{t_0}^{t} d\xi \, \langle v_i(\tau) v_j^*(\xi) \rangle. \tag{6}$$

To proceed we employ the *Leibniz rule* named after G.W. Leibniz,

$$\frac{d}{dt}\int_{a(t)}^{b(t)} d\tau f(\tau,t) = \frac{\partial b(t)}{\partial t} f[b(t),t] - \frac{\partial a(t)}{\partial t} f[a(t),t] + \int_{a(t)}^{b(t)} d\tau \frac{\partial f(\tau,t)}{\partial t}, \tag{7}$$

and Eq. (4) with (6) becomes

$$D_{ij}(t) = \frac{1}{2}\int_{t_0}^{t} d\tau [\langle v_i(t) v_j^*(\tau)\rangle + \langle v_i(\tau) v_j^*(t)\rangle]. \tag{8}$$

This exact formula relates velocity correlations to mean square displacements and can be used for diffusive as well as super- and subdiffusive transport. Furthermore, we allow complex valued positions and velocities. To use complex valued quantities is often useful if one relates particle diffusion coefficients to the magnetic correlation tensor of the turbulence (see Ref. [10]). In this case the usage of complex valued magnetic fields is crucial. The assumption of *stationary transport* (see below) was also not employed to derive Eq. (8).

A similar formula has been derived in Ref. [21]. However, these authors focused on the case $i = j$. We can express the coefficient $D_{ij}(t)$ through velocities *and* displacements by combining Eqs. (5) and (8):

$$D_{ij}(t) = \tfrac{1}{2}[\langle v_i(t)\Delta x_j^*(t)\rangle + \langle \Delta x_i(t) v_j^*(t)\rangle]. \tag{9}$$

If one knows the coefficient $D_{ij}(t)$ one can easily calculate the mean square displacement by integrating Eq. (9) over time.

Alternatively, we can define a diffusion coefficient by using

$$V_{ij}(t) := \int_{t_0}^{t} d\tau \langle v_i(t) v_j^*(\tau)\rangle, \tag{10}$$

which is equivalent to

$$V_{ij}(t) = \langle v_i(t) \Delta x_j^*(t)\rangle. \tag{11}$$

Equation (10) is the general form of the *Taylor-Green-Kubo formula* (3).

If we combine Eqs. (8) and (10), or Eqs. (9) and (11), we deduce

$$D_{ij}(t) = \frac{V_{ij}(t) + V_{ji}^*(t)}{2}. \tag{12}$$

This is an exact relation between the diffusion coefficients defined by using mean square displacements D_{ij} and the diffusion coefficients defined by using velocity correlation functions V_{ij}. It should be emphasized again that Eq. (12) can also be used for non-Markovian transport. In general we have $D_{ij} \neq V_{ij}$; i.e., the two definitions (4) and (10) are not equivalent.

III. SPECIAL CASES AND LIMITS

Here we consider special cases to simplify and to understand the relations between the different definitions of the diffusion coefficient derived above.

A. The case $i = j$

If the two indices are equal, Eq. (12) becomes

$$D_{ii}(t) = \Re\,[V_{ii}(t)]\,. \tag{13}$$

If the indices are equal the two formulas (4) and (10) provide the same result. The only difference is that, in general, $V_{ii}(t)$ can be complex valued whereas $D_{ii}(t)$ is a real number.

B. The case $i \neq j$

Now we investigate the case that the indices are different. If we consider $i = x$ and $j = y$ as an example, we derive from Eq. (12)

$$D_{xy} = \frac{V_{xy} + V_{yx}^*}{2} = D_{yx}^*. \tag{14}$$

Thus, the real parts are symmetric while the imaginary parts are antisymmetric. According to Eq. (14) we have $D_{ij} \neq V_{ij}$ if $i \neq j$. Therefore, we conclude that for the off-diagonal elements of the diffusion tensor (1), the two definitions (2) and (3) are not equivalent.

C. The case $D_{xy} = D_{yx} = 0$

If the diffusion coefficients D_{xy} and D_{yx} are zero (e.g., due to the symmetry of the physical system), we can derive from Eq. (14)

$$V_{xy} = -V_{yx}^*. \tag{15}$$

In this case the parameters V_{xy} and V_{yx} are antisymmetric. The two relations derived here are important to explain different results obtained in drift theory (see below).

D. The stationary case

In diffusion theory it is often assumed that the transport is *stationary*. In this case the velocity correlation functions depend only on the time difference; i.e., $\langle v_i(t_2)v_j^*(t_1)\rangle = \langle v_i(t_2-t_1)v_j^*(0)\rangle$ if $t_2 > t_1$. To calculate the diffusion coefficients for this case we start with Eq. (8) and employ the integral transformation $\xi = t - \tau + t_0$. We deduce

$$D_{ij}(t) = \frac{1}{2}\int_{t_0}^{t} d\xi[\langle v_i(t)v_j^*(t-\xi+t_0)\rangle + \langle v_j(t)v_i^*(t-\xi+t_0)\rangle^*], \tag{16}$$

which is still an exact relation. By additionally assuming stationary transport we derive for the special case $t_0 = 0$

$$D_{ij}(t) = \frac{1}{2}\int_{0}^{t} d\xi[\langle v_i(\xi)v_j^*(0)\rangle + \langle v_j(\xi)v_i^*(0)\rangle^*]. \tag{17}$$

In the present article we do not judge whether the assumption of stationary transport is valid for realistic scenarios or not; we just provide the correct result.

E. Stationary and Markovian transport

If we additionally assume diffusive transport, Eq. (17) can be written as

$$D_{ij} = \frac{1}{2}\int_{0}^{\infty} d\xi[\langle v_i(\xi)v_j^*(0)\rangle + \langle v_j(\xi)v_i^*(0)\rangle^*] \tag{18}$$

with $D_{ij} \equiv D_{ij}(t\to\infty)$. Again we realize that for $i \neq j$ this form does not agree with the standard form (3). If we define a diffusion coefficient by using mean square displacements—see, e.g., Eq. (2)—the standard form (3) is not correct for the off-diagonal elements of the diffusion tensor. For the diffusive case we can easily integrate Eq. (18) to find for the mean square displacements

$$\langle \Delta x_i \Delta x_j^*\rangle = (V_{ij} + V_{ji})t \tag{19}$$

with $V_{ij} \equiv V_{ij}(t\to\infty)$.

IV. RELATION TO THE DIFFUSION EQUATION

Above we have discussed two different possibilities to define a diffusion coefficient. A third way to define and use diffusion coefficients is provided by the diffusion equation.

A. Fundamental equations

According to *Fick's first law* (named after A. E. Fick) we can write

$$J_i = -\kappa_{ij}\frac{\partial f}{\partial x_j}, \tag{20}$$

where we used the *Einstein summation convention*. Furthermore, we used the *diffusion flux* J_i, the elements of the diffusion tensor κ_{ij} as above, and the distribution function $f(\vec{x},t)$ describing the probability to find the particle at the position $\vec{x}$ at time t. The latter function is normalized via

$$\int d^3x f(\vec{x},t) = 1; \tag{21}$$

i.e., the probability to find the particle somewhere in space is 1.

Since we are dealing with charged particles, we can also interpret f as charge density and J_i as the current density. Furthermore, we can employ the continuity equation

$$\frac{\partial f}{\partial t} + \frac{\partial J_i}{\partial x_i} = 0. \tag{22}$$

By combining Eqs. (20) and (22) we find the diffusion equation

$$\frac{\partial f}{\partial t} = \kappa_{ij}\frac{\partial^2 f}{\partial x_i \partial x_j}, \tag{23}$$

which is also known as *Fick's second law*. Here we assumed that the diffusion coefficients do not have a spacial dependence.

In the following we calculate the two coefficients V_{ij} and D_{ij} from the four equations discussed here. To do these derivations we assume that the function f and its derivatives are zero in the limit $x_i \to \pm\infty$ for all i.

B. The coefficient D_{ij}

In the following we calculate the mean square displacements from the diffusion equation (23). As an example we compute the mean square displacement $\langle\Delta x \Delta y\rangle$ for which we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\langle\Delta x\Delta y\rangle &= \frac{1}{2}\int d^3x\,\Delta x\Delta y\frac{\partial f}{\partial t}\\ &= \frac{1}{2}\sum_{i,j=x,y,z}\kappa_{ij}\int d^3x\,\Delta x\Delta y\frac{\partial^2 f}{\partial x_i\partial x_j}\\ &= \frac{\kappa_{xy}+\kappa_{yx}}{2}.\end{aligned} \tag{24}$$

To perform the last step we used integration by parts twice. In a similar way we can compute the other eight mean square displacements. We find the general relation

$$D_{ij} = \frac{\kappa_{ij}+\kappa_{ji}}{2} = D_{ji}, \tag{25}$$

which is correct for $i = j$ as well as $i \neq j$. However, the latter relation is only valid for the case of diffusively propagating particles. In the present article we have derived the general relation (14) which is also correct for nondiffusive and nonstationary transport and can also be used in the complex formulation of magnetic fields.

C. The coefficient V_{ij}

Now we derive a relation between the coefficients V_{ij} and the diffusion coefficients κ_{ij} occurring in the diffusion equation. We can write the current density as

$$J_i = \tilde{v}_i f. \tag{26}$$

$\tilde{v}_i = \tilde{v}_i(\vec{x},t)$ is the particles' average velocity at position $\vec{x}$ at time t. By multiplying this relation by Δx_j and by integrating the result we deduce

$$\begin{aligned}\int d^3x(\Delta x_j)\tilde{v}_i f &= \int d^3x(\Delta x_j)J_i\\ &= -\int d^3x(\Delta x_j)\kappa_{ik}\frac{\partial f}{\partial x_k}\end{aligned}$$

$$= -\kappa_{ik} \int d^3x (\Delta x_j) \frac{\partial f}{\partial x_k}$$
$$= \kappa_{ik} \int d^3x \frac{\partial (\Delta x_j)}{\partial x_k} f. \tag{27}$$

Here we used *Fick's first law* (20) and partial integration. If we use $(\partial \Delta x_j)/(\partial x_k) = \delta_{jk}$ and the normalization condition (21) we can rewrite this relation as

$$\kappa_{ij} = \langle v_i \Delta x_j \rangle. \tag{28}$$

By comparing our result with Eq. (11) we find that $V_{ij} = \kappa_{ij}$; i.e., the diffusion coefficients occurring in the diffusion equation are those defined by using velocity correlation functions—see Eq. (23). This conclusion is in agreement with the result obtained by Giacalone *et al.* (see Ref. [22]), who used a different derivation.

A more systematic derivation can be performed by introducing the velocity dependent distribution function $G = G(\vec{x},\vec{v},t)$. As a differential equation for this function one could use the *Fokker-Planck equation* (see, e.g., Ref. [10]). In this case one can write

$$\begin{aligned}
\langle v_i \Delta x_j \rangle &= \int d^3x \int d^3v v_i \Delta x_j G(\vec{x},\vec{v},t) \\
&= \int d^3x \Delta x_j \int d^3v v_i G(\vec{x},\vec{v},t) \\
&= \int d^3x \Delta x_j J_i \\
&= -\kappa_{ik} \int d^3x \Delta x_j \frac{\partial f}{\partial x_k} \\
&= \kappa_{ik} \int d^3x \delta_{jk} f \\
&= \kappa_{ij},
\end{aligned} \tag{29}$$

confirming the results obtained above and by Giacalone *et al.*

D. Solution of the diffusion equation

Here we briefly discuss the solution of the diffusion equation (23). By using standard tools of the theory of differential equations, we can easily derive the general solution of the diffusion equation

$$f(\vec{x},t) = \int d^3x' f(\vec{x}',t=0) P(\vec{x},\vec{x}',t) \tag{30}$$

with the initial distribution $f(\vec{x},t=0)$ and the *propagator*

$$P(\vec{x},\vec{x}',t) = \frac{1}{(2\pi)^3} \int d^3k e^{-\sum_{ij} \kappa_{ij} k_i k_j t + i\vec{k}\cdot(\vec{x}-\vec{x}')}. \tag{31}$$

If we assume that the particle has a well-defined initial position $\vec{x} = 0$ we can use

$$f(\vec{x},t=0) = \delta(\vec{x}) \tag{32}$$

with the *Dirac delta function* $\delta(x)$. In this case the solution of the diffusion equation has the form

$$f(\vec{x},t) = \frac{1}{(2\pi)^3} \int d^3k e^{-\sum_{ij} \kappa_{ij} k_i k_j t + i\vec{k}\cdot\vec{x}}. \tag{33}$$

Below we will simplify these results by assuming axial symmetry.

E. The diffusion tensor for axial symmetry

In the physics of charged particle diffusion in magnetized plasmas it is often assumed that turbulent magnetic fields are superposed by a mean magnetic field $\vec{B}_0$. In the present paper we assume that the (constant) mean magnetic field points in the z direction so that $\vec{B}_0 = B_0 \vec{e}_z$. Furthermore, we assume that the turbulence and therewith the whole physical system is axisymmetric with respect to the mean field. In this special case the diffusion tensor (1) has the general form

$$(\kappa_{ij}) = \left\{ \begin{matrix} \kappa_\perp & \kappa_A & 0 \\ -\kappa_A & \kappa_\perp & 0 \\ 0 & 0 & \kappa_\parallel \end{matrix} \right\}. \tag{34}$$

It is straightforward to prove that this form is invariant under arbitrary rotations about the z axis, i.e., $\kappa_{ij} = R^T_{il} \kappa_{lm} R_{mj}$, where we used the *rotation matrix* R_{ij}. The parameters used in Eq. (34) are the perpendicular diffusion coefficient $\kappa_\perp$, the parallel diffusion coefficient $\kappa_\parallel$, and the drift coefficient κ_A.

F. The diffusion equation for axial symmetry

In the case of axial symmetry we obtain for the diffusion equation

$$\frac{\partial f}{\partial t} = \kappa_\parallel \frac{\partial^2 f}{\partial z^2} + \kappa_\perp \left[\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} \right], \tag{35}$$

and the solution of the diffusion equation (33) has the form

$$\begin{aligned}
f(\vec{x},t) &= \frac{1}{(2\pi)^3} \int d^3k e^{-\kappa_\parallel k_\parallel^2 t - \kappa_\perp k_\perp^2 t + i\vec{k}\cdot\vec{x}} \\
&= \frac{1}{(4\pi t \kappa_\perp)\sqrt{4\pi t \kappa_\parallel}} e^{-\frac{x^2+y^2}{4\kappa_\perp t} - \frac{z^2}{4\kappa_\parallel t}}.
\end{aligned} \tag{36}$$

Often this form is employed to develop nonlinear diffusion theories of energetic particles (see, e.g., Ref. [10]). Obviously the drift terms do not influence the solution of the diffusion equation.

G. The diffusive flux for axial symmetry

By using *Fick's first law* (20) we can easily compute the flux vector. With the solution (36) and by using $\kappa_{xy} = -\kappa_A = -\kappa_{yx}$ we find after straightforward algebra

$$\begin{aligned}
J_x &= \left(\frac{x}{2t} - \frac{\kappa_A}{\kappa_\perp} \frac{y}{2t} \right) f(\vec{x},t), \\
J_y &= \left(\frac{y}{2t} + \frac{\kappa_A}{\kappa_\perp} \frac{x}{2t} \right) f(\vec{x},t), \\
J_z &= \frac{z}{2t} f(\vec{x},t).
\end{aligned} \tag{37}$$

Clearly we can see the influence of the drift coefficients on the diffusive flux.

H. The nonaxisymmetric case

Sometimes it is assumed that for the case in which the physical system is not axisymmetric we have the more general form

$$(\kappa_{ij}) = \begin{Bmatrix} \kappa_{xx} & \kappa_{xy} & 0 \\ \kappa_{yx} & \kappa_{yy} & 0 \\ 0 & 0 & \kappa_{zz} \end{Bmatrix}. \tag{38}$$

In this case the diffusion equation (23) becomes

$$\frac{\partial f}{\partial t} = \kappa_{xx}\frac{\partial^2 f}{\partial x^2} + \kappa_{yy}\frac{\partial^2 f}{\partial y^2} + (\kappa_{xy}+\kappa_{yx})\frac{\partial^2 f}{\partial x \partial y} + \kappa_{zz}\frac{\partial^2 f}{\partial z^2}. \tag{39}$$

In this case we can use Eq. (25) to find for the diffusion equation

$$\frac{\partial f}{\partial t} = D_{xx}\frac{\partial^2 f}{\partial x^2} + D_{yy}\frac{\partial^2 f}{\partial y^2} + (D_{xy}+D_{yx})\frac{\partial^2 f}{\partial x \partial y} + D_{zz}\frac{\partial^2 f}{\partial z^2} \tag{40}$$

with $D_{xy} = D_{yx}$. Therefore, we conclude that for the solution of the diffusion equation it does not matter whether we use definition (2) or (3) for the diffusion coefficients. The solution is the same. This statement is very important since the solution of Eq. (40) is often employed to model the nonlinear transport of energetic particles. As shown in the present paper this form is correct. Furthermore, the propagator (31) can be written as

$$P(\vec{x},\vec{x}',t) = \frac{1}{(2\pi)^3}\int d^3k e^{-\sum_{ij} D_{ij}k_i k_j t + i\vec{k}\cdot(\vec{x}-\vec{x}')} \tag{41}$$

if the form (38) holds. Thus, for modeling the nonlinear transport of energetic particles, we can also use D_{ij} instead of $\kappa_{ij} = V_{ij}$. The difference between the two diffusion coefficient is only important if the diffusive flux J_i is calculated.

V. EXAMPLE: DRIFT THEORY OF COSMIC PARTICLES

The flux of cosmic rays incident on the Earth's upper atmosphere is modulated by the solar wind. A fundamental problem in the theory of cosmic ray modulation is the description of the drift coefficient (see Ref. [20]). Drift theory is a good example of the applicability of the results derived above. The form (34) can be seen as standard form in cosmic ray diffusion theory (see, e.g., Refs. [23–26]). Here, the diagonal elements describe diffusion of particles parallel and perpendicular to the mean magnetic field. The off-diagonal, antisymmetric terms $\pm\kappa_A$ describe effects of gradient and curvature drifts. Whereas progress has been achieved in the theory of parallel and perpendicular diffusion (see, e.g., Refs. [10] and [27]), a widely accepted theory of cosmic ray drifts is still not available.

Burger and Visser (see Ref. [20]) have pointed out that one can find different results for κ_{xy} and κ_{yx} in the literature which contradict each other. Some authors (see Refs. [28] and [29]) derived $\kappa_{xy} = \kappa_{yx} = 0$ whereas others (see Refs. [30] and [31]) found $\kappa_{xy} = -\kappa_{yx} \neq 0$. Candia and Roulet (see Ref. [30]), for instance, have used the standard *TGK formula* (3), whereas other authors used Eq. (2). By taking into account the results of the present paper, the contradiction between those previous results is evident. Below we review previous approaches for the drift coefficient.

A. The unperturbed orbit

The simplest description of the particle motion can be achieved by neglecting the turbulent magnetic field. In this case the particle trajectory is a perfect helix in the perpendicular direction whereas the parallel motion occurs with constant velocity. By solving the *Newton-Lorentz equation* for this simple case we find for the particle mean square displacements

$$\begin{aligned} \Delta x(t) &= \frac{v_x(0)}{\Omega}\sin(\Omega t) + \frac{v_y(0)}{\Omega}[1-\cos(\Omega t)], \\ \Delta y(t) &= \frac{v_x(0)}{\Omega}[\cos(\Omega t)-1] + \frac{v_y(0)}{\Omega}\sin(\Omega t), \end{aligned} \tag{42}$$

and for the velocity components

$$\begin{aligned} v_x(t) &= v_x(0)\cos(\Omega t) + v_y(0)\sin(\Omega t), \\ v_y(t) &= -v_x(0)\sin(\Omega t) + v_y(0)\cos(\Omega t). \end{aligned} \tag{43}$$

Here we have used the gyrofrequency Ω and the initial velocity components in the x and y directions, respectively. In the following we will compute the coefficients V_{xy} and V_{yx} by using Eq. (11) for real valued displacements and velocities. In the unperturbed case we interpret the average operator $\langle\ldots\rangle$ as average over all possible initial velocities; i.e.,

$$\langle\ldots\rangle \equiv \frac{1}{(2v)^2}\int_{-v}^{+v} dv_x \int_{-v}^{+v} dv_y. \tag{44}$$

We derive

$$V_{xy} = -V_{yx} = \frac{v^2}{3\Omega}[1-\cos(\Omega t)]. \tag{45}$$

If we neglect oscillations (e.g., by averaging over one gyroperiod) we find $V_{xy} = -V_{yx} = v^2/(3\Omega)$. The latter result is known as the *weak scattering limit* (WSL) and has been derived earlier from the unperturbed orbit (see, e.g., Ref. [20]). According to those results we even find a finite drift coefficient κ_A if there is no turbulence. The WSL is an exact result for the case in which there is no turbulence. Therefore, it provides a useful benchmark to test more general diffusion theories. Each theory for charged particle drifts should provide the WSL in the appropriate limit. This limit, however, is valid for the coefficients $V_{xy} = -V_{yx}$. For the diffusion coefficients defined by using mean square displacements, we find $D_{xy} = D_{yx} = 0$. The same calculations can be performed for the diagonal elements of the diffusion tensor. By combing Eqs. (42)–(44) and by averaging over a gyroperiod we can easily derive $V_{xx} = V_{yy} = 0$ for the unperturbed case.

B. The Bieber and Matthaeus model

A *heuristic approach* for perpendicular diffusion and drifts has been developed by Bieber and Matthaeus (see Ref. [26]). The latter authors started with the motion of a particle in a constant mean magnetic field without turbulence as described above. Then they multiplied the unperturbed velocity correlation functions with exponential factors to describe the scattering of particles and therewith the decorrelation from the unperturbed orbit. They used the *Ansatz*

$$\langle v_x(t) v_y(0) \rangle = \frac{v^2}{3} \sin(\Omega t) e^{-\omega t} = -\langle v_y(t) v_x(0) \rangle. \quad (46)$$

Here Ω is the gyrofrequency of the particle and ω is an (unknown) scattering frequency describing the interaction with magnetic turbulence. According to Eq. (18) the diffusion coefficient defined by mean square displacements yields zero for this model. If we use Eq. (3), however, we get

$$V_{xy} = \frac{v^2}{3} \frac{\Omega}{\Omega^2 + \omega^2} = -V_{yx}. \quad (47)$$

For $\omega \ll \Omega$ we can easily obtain the WSL. A more complete description of drifts and applications in the theory of solar modulation can be found in Ref. [20].

VI. SUMMARY AND CONCLUSION

We can clearly see that *what we get* depends on how we define and calculate the drift coefficient. Equations (2) and (3) are *not* equivalent for the off-diagonal elements. The coefficients used in the diffusion equation correspond to those defined by velocity correlations and not by mean square displacements. For the diagonal elements the three definitions are equivalent—see Eq. (13) of the present paper.

As an example we have considered the drift coefficient of cosmic particles propagating through the solar system. As discussed by Burger and Visser (see Ref. [20]) previous results for the drift coefficients contradict each other. Some authors found $\kappa_{xy} = \kappa_{yx}$ whereas other investigators found $\kappa_{xy} = -\kappa_{yx}$. This disagreement caused some confusion and discussion about the correctness of the different approaches and calculations. The reason for those differences is that definition (2) of the diffusion coefficient and the *Kubo formula* (3) are not equivalent for drifts.

In some cases, however, one is just interested in the solution of the diffusion equation. In this case the replacement $\kappa_{ij} \to D_{ij}$ is allowed. This is especially the case if one tries to formulate a nonlinear theory for particle transport (see, e.g., Ref. [10]). If one is interested in the diffusion flux, however, it is essential to distinguish between the parameters $\kappa_{ij} = V_{ij}$ and D_{ij}. This difference is important in the theory of solar modulation.

The results of the present paper are fundamental and not restricted to the propagation of energetic particles in the solar system. In any two or three dimensional system where we have a stochastic motion of particles, we can use a set of diffusion coefficients to describe the motion of particles. A further example for a stochastic process is the wandering of magnetic field lines in turbulence (see, e.g., Refs. [32] and [33]). For such processes the results of the present paper could also be important. In general, we can have nonvanishing off-diagonal diffusion coefficients in such systems. The present paper explains how such coefficients can be calculated and that special care is required if one tries to compute the drift coefficient.

[1] R. Brown, Philos. Mag. **4**, 161 (1828).
[2] A. Einstein, Ann. Phys. **17**, 549 (1905).
[3] S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943).
[4] R. Balescu, *Transport Processes in Plasmas: 2. Neoclassical Transport Theory* (North-Holland, Amsterdam, 1988).
[5] R. Balescu, *Aspects of Anomalous Transport in Plasmas* (Institute of Physics Publishing, Bristol, 2005).
[6] A. Shalchi and A. Dosch, Phys. Rev. D **79**, 083001 (2009).
[7] R. J. Bickerton, Plasma Phys. Controlled Fusion **39**, 339 (1997).
[8] J. Wesson, *Tokamaks* (Clarendon, Oxford, 2004).
[9] R. Schlickeiser, *Cosmic Ray Astrophysics* (Springer-Verlag, Berlin, 2002).
[10] A. Shalchi, *Nonlinear Cosmic Ray Diffusion Theories*, Astrophysics and Space Science Library, Vol. 362 (Springer, Berlin, 2009).
[11] J. Klafter, A. Blumen, and M. F. Shlesinger, Phys. Rev. A **35**, 3081 (1987).
[12] G. M. Zaslavskii, R. Z. Sagdeev, D. K. Chaikovskii, and A. A. Chernikov, JETP Lett. **68**, 995 (1989).
[13] G. Zimbardo and P. Veltri, Phys. Rev. E **51**, 1412 (1995).
[14] R. Sánchez, B. A. Carreras, and B. Ph. van Milligen, Phys. Rev. E **71**, 011111 (2005).
[15] G. Zimbardo, P. Pommois, and P. Veltri, Astrophys. J. **639**, L91 (2006).
[16] A. Shalchi and I. Kourakis, Astron. Astrophys. **470**, 405 (2007).
[17] G. I. Taylor, Proc. London Math. Soc. **20**, 196 (1922).
[18] M. S. Green, J. Chem. Phys. **19**, 1036 (1951).
[19] R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957).
[20] R. A. Burger and D. J. Visser, Astrophys. J. **725**, 1366 (2010).
[21] A. Dosch, A. Shalchi, and B. Weinhorst, Adv. Space Res. **44**, 1326 (2009).
[22] J. Giacalone, J. R. Jokipii, and J. Kóta, in *Proc. 26th International Cosmic Ray Conference*, edited by D. Kieda, M. Solamon, and B. Dingus (University of Utah, Salt Lake City, 1999), Vol. 7, p. 37.
[23] L. J. Gleeson, Planet. Space Sci. **17**, 31 (1969).
[24] M. A. Forman, Astrophys. Space Sci. **49**, 83 (1977).
[25] J. R. Jokipii, E. H. Levy, and W. B. Hubbard, Astrophys. J. **213**, 861 (1977).
[26] J. W. Bieber and W. H. Matthaeus, Astrophys. J. **485**, 655 (1997).
[27] A. Shalchi, Astrophys. J. **720**, L127 (2010).
[28] J. A. le Roux and G. M. Webb, Astrophys. J. **667**, 930 (2007).
[29] B. Weinhorst, A. Shalchi, and H. Fichtner, Astrophys. J. **677**, 671 (2008).
[30] J. Candia and E. Roulet, J. Cosmol. Astropart. Phys. **10**, 007 (2004).
[31] J. Minnie, J. W. Bieber, W. H. Matthaeus, and R. A. Burger, Astrophys. J. **670**, 1149 (2007).
[32] W. H. Matthaeus, P. C. Gray, D. H. Pontius Jr., and J. W. Bieber, Phys. Rev. Lett. **75**, 2136 (1995).
[33] A. Shalchi and I. Kourakis, Phys. Plasmas **14**, 092903 (2007).